

Some exact stationary state solutions of a nonlinear Dirac equation in 2+1 dimensions

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Abstract

Graphene's honeycomb lattice structure is quite remarkable in the sense that it leads, in the long wavelength limit, to a massless Dirac equation description of nonrelativistic quasiparticles associated with electrons and holes present in the two dimensional crystallite. In the case of cold bosonic atoms trapped in a honeycomb optical lattice, Haddad and Carr (2009) have recently shown, by taking into account binary contact interactions, that the dynamics of these Bose-Einstein condensates is governed by a nonlinear Dirac equation (NLDE). In this paper, we study exact stationary solutions of such a NLDE. After proving that the energy eigenvalues are real, we show that the sum of orbital angular momentum and pseudospin angular momentum normal to the crystal commutes with the nonlinear Hamiltonian whenever magnitudes of the pseudospin components do not depend on the polar angle ϕ . We obtain some exact stationary and localized solutions of the NLDE.

I. INTRODUCTION

Graphene, peeled off from bulk graphite by means of micromechanical cleavage technique, is a zero-gap semiconductor [1,2]. Being a monolayer of carbon atoms arranged in a planar hexagonal lattice structure in which charge carriers travel distances that are thousand times the lattice spacing without being subjected to any scattering, graphene helped in establishing that stable two dimensional crystals do exist, contrary to what one expects from thermodynamic instability arguments put forward by Landau, Peierls and Mermin in the past [3,4].

For wavelengths much larger than the lattice size, charged quasiparticles in the honeycomb lattice satisfy a massless Dirac equation [5-7],

$$i\hbar \frac{\partial \psi}{\partial t} = -i\hbar v_F (\vec{\sigma} \cdot \nabla) \psi \quad (1)$$

where,

$$\begin{aligned} \psi &= \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} \\ \nabla &= \hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} \\ \vec{\sigma} &= \hat{i} \sigma_x + \hat{j} \sigma_y \end{aligned}$$

and $v_F \approx 0.01 c$ represents the Fermi speed. The components ψ_A and ψ_B are bi-component spinors describing spin-half charge carriers, while subscripts A and B refer to the two inequivalent sites A and B of the sublattice forming the hexagonal structure, representing pseudospin degrees of freedom. The associated Clifford algebra,

$$\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2 \eta^{\mu\nu}, \quad \mu, \nu = 0, 1, 2$$

is satisfied by,

$$\gamma^0 = \sigma_z, \gamma^1 = \sigma_z \sigma_x, \gamma^2 = \sigma_z \sigma_y .$$

Relativistic quantum features like *zitterbewegung* and Klein paradox, which so far have been confined to the domain of quantum electrodynamics, make their appearance in the context of subrelativistic charge carriers in graphene because of eq.(1) [8].

In an interesting recent paper, Haddard and Carr have studied weakly interacting bosonic atoms anchored to a planar honeycomb optical lattice [9]. The quantum many body theory

of this system is described by a Hamiltonian,

$$\hat{H} = \int \int \Phi^\dagger \left(\frac{-\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right) \Phi \, dx \, dy + \lambda \int \int \Phi^\dagger \Phi^\dagger \Phi \Phi \, dx \, dy \quad (2)$$

where the field of identical atoms each having mass m is represented by a complex scalar field operator $\Phi(\vec{r}, t)$. The potential $V(\vec{r})$ encapsulates interactions of atoms with electromagnetic fields from laser beams responsible for pinning the atoms to a two dimensional optical lattice. The second term in eq.(2) arises because of binary contact interaction between atoms, λ being a coupling constant proportional to the s-wave scattering length.

As a result of both the planar honeycomb lattice structure as well as the presence of a contact interaction term in eq.(2), the dynamics of Bose-Einstein condensate (BEC) in this case is described by a nonlinear Dirac equation,

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}(\psi)\psi = -i\hbar c_s (\vec{\sigma} \cdot \nabla) \psi + M(\psi)\psi \quad (3)$$

where $c_s \approx \text{few } cm \, s^{-1}$ is an effective BEC sound speed in the planar lattice, and ψ represents the state of BEC,

$$\psi = \begin{pmatrix} \psi_A(x, y, t) \\ \psi_B(x, y, t) \end{pmatrix}$$

with ψ_A and ψ_B now being scalar wavefunctions representing spatio-temporal and pseudospin degrees of freedom for the bosonic atoms, while $M(\psi)$ embodies the nonlinearity arising out of s-wave scatterings,

$$M(\psi) = U \begin{pmatrix} |\psi_A|^2 & 0 \\ 0 & |\psi_B|^2 \end{pmatrix}$$

U being the interaction energy [9].

From eq.(3), one can straight away obtain the conservation of probability current,

$$\frac{1}{c} \frac{\partial P}{\partial t} + \nabla \cdot \vec{J} = 0 \quad (4)$$

where,

$$P \equiv \psi^\dagger \psi = \psi_A^* \psi_A + \psi_B^* \psi_B$$

and,

$$\vec{J} \equiv c_s \psi^\dagger \vec{\sigma} \psi$$

Because of eq.(4), one may normalize the BEC wavefunction,

$$\int \int P \, dx \, dy = \int \int (|\psi_A|^2 + |\psi_B|^2) \, dx \, dy = 1 \quad (5)$$

II. DISPERSION RELATION, INNER PRODUCT AND ENERGY

In order to study dispersion relation in NLDE, we substitute the following plane wave form in eq.(3),

$$\psi = \begin{pmatrix} C_A e^{i(k_x x + k_y y - \omega t)} \\ C_B e^{i(k_x x + k_y y - \omega t)} \end{pmatrix}$$

that entails,

$$(\omega - \frac{U}{\hbar} |C_B|^2) C_B = c_s (k_x + i k_y) C_A \quad (6a)$$

and,

$$(\omega - \frac{U}{\hbar} |C_A|^2) C_A = c_s (k_x - i k_y) C_B \quad (6b)$$

Assuming box-normalization for ψ on a square of side length L , one obtains from eq.(5),

$$|C_A|^2 + |C_B|^2 = \frac{1}{L^2} \quad (7)$$

Making use of eqs. (6a), (6b) and (7), we arrive at,

$$|C_A|^2 = \frac{1}{2L^2} \left(1 \pm \sqrt{1 - \frac{4L^2}{U} \left(\hbar\omega - \hbar^2 \Delta^2 \frac{L^2}{U} \right)} \right) \quad (8)$$

where,

$$\Delta^2 \equiv \omega^2 - c_s^2 (k_x^2 + k_y^2). \quad (9)$$

Reality of $|C_A|^2$ requires,

$$\frac{\hbar\omega}{U} \leq \frac{1}{4L^2} + \frac{\hbar^2 L^2 \Delta^2}{U^2} \quad (10)$$

Therefore, for $U > 0$, eq.(10) implies that if,

$$\hbar\omega \leq \frac{U}{4L^2} + \frac{\hbar^2 L^2 \Delta^2}{U} \quad (11)$$

plane wave solutions of eq.(3), corresponding to ‘massive modes’ with tiny mass $\sqrt{\frac{\hbar^2 \Delta^2}{c^4}}$, are possible.

If the inner product of two BEC states ψ and χ is defined in the usual manner as,

$$(\psi, \chi) = \int \int \psi^\dagger \chi \, dx \, dy \quad (12)$$

one can trivially verify that,

$$(M(\psi)\chi, \psi) = (\chi, M(\psi)\psi) \quad (13)$$

which entails,

$$(\hat{H}(\psi)\chi, \psi) = (\chi, \hat{H}(\psi)\psi) \quad (14)$$

since $-i\hbar(\vec{\sigma} \cdot \nabla)$ is self-adjoint.

Therefore, if ψ_E is an energy eigenstate so that,

$$\hat{H}(\psi_E)\psi_E = E\psi_E \quad (15)$$

then substituting ψ_E in place of χ and ψ in eq.(14), leads to the result that E is real.

However, if

$$\hat{H}(\psi_i)\psi_i = E_i\psi_i, \quad i = 1, 2$$

then, in general, ψ_1 and ψ_2 are not mutually orthogonal for non-zero U .

(It must be pointed out here that technically we should not be using terms like eigenvalues and eigenstates since we are dealing with a nonlinear operator $\hat{H}(\psi)$. But since these terms have entered the common parlance of quantum theory, we will continue to use them.)

Suppose $U = 0$ so that the Hamiltonian appearing in eq.(3) is just $-i\hbar c_s(\vec{\sigma} \cdot \nabla)$. Then, it is interesting to observe that the orbital angular momentum normal to the planar lattice does not commute with the Hamiltonian,

$$[\hat{L}_z, -i\hbar\vec{\sigma} \cdot \nabla] = \hbar^2 \left(\sigma_x \frac{\partial}{\partial y} - \sigma_y \frac{\partial}{\partial x} \right) \quad (16)$$

Now, since,

$$[\sigma_z, -i\hbar\vec{\sigma} \cdot \nabla] = -2\hbar \left(\sigma_x \frac{\partial}{\partial y} - \sigma_y \frac{\partial}{\partial x} \right) \quad (17)$$

we can get using eqs.(16) and (17),

$$[L_z + \frac{\hbar}{2}\sigma_z, -i\hbar\vec{\sigma} \cdot \nabla] = 0. \quad (18)$$

suggesting that $L_z + \frac{\hbar}{2}\sigma_z$ plays the role of total angular momentum. But this is puzzling as $\vec{\sigma}$ appearing in eq.(3) reflects only pseudospin degrees of freedom. In the context of graphene, using much more extensive arguments, Mecklenburg and Regan have recently made a case for identifying pseudospin with intrinsic spin angular momentum [10]. Although eq.(3) describes a bosonic system, the pseudospin degrees arising out of sites A and B of a two dimensional honeycomb lattice appear to induce a half-integral spin angular momentum for the BEC when $U = 0$.

III. LOCALIZED STATIONARY SOLUTIONS

In this section, we look for energy eigenfunctions of the NLDE whose magnitudes fall with radial distance. It is convenient to switch to polar coordinates (r, ϕ) , so that a stationary state solution $\psi_E(r, \phi, t)$ of the NLDE has the form,

$$\psi_E = e^{-\frac{i}{\hbar}Et} \psi(r, \phi)$$

where,

$$\psi(r, \phi) = \begin{pmatrix} \psi_A(r, \phi) \\ \psi_B(r, \phi) \end{pmatrix}$$

satisfies the time independent NLDE,

$$E\psi_A = -i\hbar c_s e^{-i\phi} \left(\frac{\partial \psi_B}{\partial r} - \frac{i}{r} \frac{\partial \psi_B}{\partial \phi} \right) + U|\psi_A|^2 \psi_A \quad (19)$$

$$E\psi_B = -i\hbar c_s e^{i\phi} \left(\frac{\partial \psi_A}{\partial r} + \frac{i}{r} \frac{\partial \psi_A}{\partial \phi} \right) + U|\psi_B|^2 \psi_B, \quad (20)$$

E being the energy.

In polar coordinates, the orbital angular momentum is simply $\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}$. Therefore,

$$[\hat{L}_z, M(\psi)] = 0$$

only when both $|\psi_A|^2$ and $|\psi_B|^2$ are independent of the angle ϕ . Since $[\sigma_z, M(\psi)]$ vanishes for all ψ , in order that $\hat{L}_z + \frac{\hbar}{2}\sigma_z$ commutes with $\hat{H}(\psi)$, the two components of ψ must take the following form,

$$\psi_A(r, \phi) = R_A(r) e^{i\Theta_A(r, \phi)} \quad (21)$$

and,

$$\psi_B(r, \phi) = R_B(r) e^{i\Theta_B(r, \phi)} \quad (22)$$

We seek solutions that are simultaneous eigenfunctions of the nonlinear Hamiltonian and the total angular momentum normal to the optical lattice. So, making use of eqs.(21) and (22) in eqs.(19) and (20) we find,

$$\Theta_A(r, \phi) = (l - \frac{1}{2})\phi + f_A(r) \quad (23)$$

$$\Theta_B(r, \phi) = (l + \frac{1}{2})\phi + f_B(r) \quad (24)$$

for $l = 0, 1, 2, \dots$, while the radial parts satisfy,

$$ER_A = -i\hbar c_s e^{i(f_B - f_A)} \left(\frac{dR_B}{dr} + iR_B \frac{df_B}{dr} + \frac{R_B}{r} \left(l + \frac{1}{2} \right) \right) + UR_A^3 \quad (25)$$

$$ER_B = -i\hbar c_s e^{-i(f_B - f_A)} \left(\frac{dR_A}{dr} + iR_A \frac{df_A}{dr} - \frac{R_A}{r} \left(l - \frac{1}{2} \right) \right) + UR_B^3 \quad (26)$$

When $R_A = R_B$, using the reality of energy E , one can deduce from eqs. (25) and (26) the following class of exact solutions,

$$R_A = R_B = Kr^{-1/2} \quad (27)$$

$$f_B(r) = f_A(r) + Q \quad (28)$$

where,

$$Q \equiv \sin^{-1} \left(-\frac{l\hbar c_s}{UK^2} \right), \quad (29)$$

with K being the normalization constant.

If $l = 0$, we get,

$$f_A(r) = \frac{(-1)^n}{\hbar c_s} [Er - UK^2 \ln r] + K_1 \quad (30)$$

and,

$$f_B(r) = f_A(r) + n\pi \quad (31)$$

where K_1 is an arbitrary real constant.

For other integral values of l , eqs. (25)-(27) demand vanishing of energy eigenvalue along with,

$$f_A(r) = -\frac{UK^2}{\hbar c_s} \cos Q \ln r + K_2, \quad (31)$$

where Q is given by eq.(29) and K_2 is a real constant.

If we normalize the wavefunction over a circular region of radius L , the constant K gets fixed to,

$$K = \frac{1}{\sqrt{4\pi L}}$$

To summarize our results, we have obtained exact solutions of a nonlinear Dirac equation given by eq.(3) for the case $|\psi_A| = |\psi_B|$ that correspond to definite energy and angular momentum normal to the plane of the optical lattice. The position probability density for these solutions decrease as r^{-1} . While the s-wave solution can have any value of energy, solutions with $l = 1, 2, \dots$ are static in nature since $E = 0$.

What is interesting is that the planar honeycomb lattice not only leads to a massless nonlinear Dirac equation description of the BEC but also makes the pseudospin degrees of freedom appear as half-integral spin degrees in a purely bosonic system (also see [10]).

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